

N-Butylnitrite  
544-16-1 | DTXSID8049418

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.09 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 5.43e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>3-Mercaptopropanoic acid</div> <div>Measured: 5.10</div> <div>Predicted: 5.30e-02</div>	<div>Image not found</div> <div>Diethoxymethane</div> <div>Measured: 3.97</div> <div>Predicted: 50.4</div>	<div>Image not found</div> <div>N-Methylcarbamic acid, ethyl ester</div> <div>Measured: 8.92e-01</div> <div>Predicted: 1.51</div>
<div>Image not found</div> <div>2,4-Pentanedione</div> <div>Measured: 1.36</div> <div>Predicted: 3.07</div>	<div>Image not found</div> <div>Nitralin</div> <div>Measured: 7.61</div> <div>Predicted: 1.77e-08</div>	